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A fully implicit finite element method for bidomain models of cardiac electromechanics

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ABSTRACT

We propose a novel, monolithic, and unconditionally stable finite element algorithm for the bidomain-based approach to cardiac electromechanics. We introduce the transmembrane potential, the extracellular potential, and the displacement field as independent variables, and extend the common two-field bidomain formulation of electrophysiology to a three-field formulation of electromechanics. The intrinsic coupling arises from both excitation-induced contraction of cardiac cells and the deformation-induced generation of intra-cellular currents. The coupled reaction–diffusion equations of the electrical problem and the momentum balance of the mechanical problem are recast into their weak forms through a conventional isoparametric Galerkin approach. As a novel aspect, we propose a monolithic approach to solve the governing equations of excitation–contraction coupling in a fully coupled, implicit sense. We demonstrate the consistent linearization of the resulting set of non-linear residual equations. To assess the algorithmic performance, we illustrate characteristic features by means of representative three-dimensional initial-boundary value problems. The proposed algorithm may open new avenues to patient specific therapy design by circumventing stability and convergence issues inherent to conventional staggered solution schemes.

1. Introduction

The past two decades have seen tremendous progress in the computational modeling of the heart [23,24]. Efficient computational tools for the assistance of patient specific treatment of cardiac disorders is of great scientific and socio-economical interest [3]. We have come to appreciate that these tools can provide access to regionally varying quantities such as wall strains or stresses, which are virtually impossible to measure in the beating heart [30,58]. Although tremendous effort has been devoted to understand the coupled electrical and mechanical response of the heart, most existing algorithms solve the electrical and mechanical fields in a decoupled way, typically by using different discretization techniques in time and space for the individual fields [27]. Historically, the biochemical response has been modeled by biophysicists [12,21,36], the electrical response by electrical engineers [2,7], the mechanical response by mechanical engineers [8,20], and the clinical response by clinicians [5,25]. The lack of cross-talk between the individual disciplines has hampered the creation of a unified, robust and stable, fully coupled multiscale-multifield solution strategy.

The bidomain equations represent a homogenization of the intracellular and extracellular medium [33,59]. The coupled bidomain equations of electrophysiology have been traditionally solved through staggered solution schemes. The solution of the parabolic and elliptic part of the the bidomain equations via operator splitting follows a common recipe: In the first step, the elliptic part is solved for a constant transmembrane potential ϕ. In the second step, the parabolic part is solved for a constant external potential ϕ_e [56,61,63]. Apparently, the operator splitting simplifies the coupled nonsymmetric set of equations with symmetric and smaller subsystems at the expense of computation time and stability [15,48]. The strong coupling due to steep excitation wavefront causes significant stability issues and renders the staggered algorithms *computationally inefficient* and *expensive*. This fact motivated the intense study of the *monodomain* equation, which is obtained through the proportionality assumption between the conduction tensors of the intra- and extracellular domains of the bidomain model. This assumption reduces the coupled bidomain equations to a single parabolic reaction–diffusion equation, which

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a priori satisfies the elliptic part of the bidomain model. It should be mentioned that the simplified monodomain model of electrophysiology is incapable of modeling the externally applied shock-induced polarization due to nonproportional conductances between the intra- and extracellular spaces and typically mispredicts the velocity of the front depolarization wave [44]. This limits use of the monodomain model in defibrillation simulations. An alternative remedy for the solution of the bidomain equations is the improvement of the solution algorithms. To this end, semi-implicit integration methods where the local and global field variables are updated through explicit and semi-implicit methods [26], predictor–corrector type time stepping algorithms [61,63,54] and three-step operator splitting techniques are employed in order to improve the stability and accuracy of solution algorithms [62]. Various preconditioning strategies, e.g. *symmetric successive over relaxation* [41], *block Jacobi* [14,61], *block triangular monodomain* [15], *multigrid* [40,41,56,48] and *multilevel (hybrid) Schwarz* methods have been devised for the linearized set of equations resulting from operator splitting algorithms [35,49–51]. A *hybridomain* model, which is adapted based on a posteriori error estimator to either bi- or monodomain, is introduced in order to improve the comptutational efficiency of the semi-implicit integration [34].

Various anisotropic continuum based models [22,37] and finite element formulations [16] are developed for the passive mechanical response of the heart. The three-dimensional structure of the heart can be constructed from segmented MRI data [43,45] and the myofiber orientation in the heart can be obtained by anisotropic least square filtering followed by fiber and sheet tracking techniques applied to the Diffusion Tensor Magnetic Resonance Imaging data of the excised human heart [46]. Operator splitting schemes based on monodomain electrophysiology have been proposed for the electromechanical excitation–contraction problem in [39,47,60,38]. These approaches combine a finite difference method to integrate the excitation equations, with a Galerkin finite element method to solve the equations governing tissue mechanics.

Current state-of-the-art electrophysiological and passive mechanical models enable researchers to explore arrhythmogenesis at the organ level. In order to enable the use of these models for patient-specific therapy design, we still lack *efficient numerical methods*. At this point, it is noteworthy to say that the above mentioned procedures do not heal the inherent instability issues associated with both *decoupled semi-explicit* solution strategies and *nonconsistent* linearization of the variational formulation. Recently, we have proposed a unified, unconditionally stable, finite element formulation based on a Galerkin-type variational formulation for the monodomain electrophysiology [17], bidomain electrophysiology [9] and monodomain based two-field electromechanics [18]. The unconditional stability and the quadratic convergence of the formulations results from the fully implicit backward Euler scheme employed for the integration of the global and local field variables and the consistent linearization of the residual terms obtained from the weak form.

In this follow up work, we extend the monolithic schemes proposed for the bidomain electrophysiology [9] and the two-field electromechanics [18] to three-field excitation contraction coupling [10]. The proposed structure is inherently modular and can be easily generalized to the three-field electro-chemistry [64], the four-field photo-electro-chemistry [1], or the four-field chemo-electro-mechanics of the heart. Unlike existing discretization schemes, which are most powerful on regular grids [6], the proposed finite element based discretization can be applied to arbitrary geometries with arbitrary initial and boundary conditions. It is easily applicable to medical-image based patient-specific geometries [29,42,66]. The resulting algorithm provides an unconditionally stable and geometrically flexible framework, which opens possibilities for the analysis of defibrillation phenomena and their impact on the electromechanical behavior of heart tissue. We demonstrate the performance of the proposed approach through a coupled electromechanical analysis of spiral wave initiation in a slice of cardiac tissue and excitation contraction of a three-dimensional generic biventricular heart model. The computational cost of the model in comparison to monolithic monodomain electromechanics formulation is commented.

This manuscript is organized as follows: In Section 2, we introduce the governing equations of cardiac electromechanics consisting of the bidomain model of electrophysiology and the quasi-static linear momentum balance. Section 3 is devoted to the derivation of the weak forms of the field equations, their consistent linearization, and their spatio-temporal discretization. Therein, we apply the finite element method in space and a backward Euler type finite difference scheme in time. In Section 4, we specify the constitutive equations for the underlying source and flux terms, and derive the corresponding consistent algorithmic tangent moduli. Section 5 is concerned with numerical examples demonstrating the distinctive performance of the proposed approach. We conclude the manuscript with closing remarks in Section 6.

2. Governing equations of the cardiac electromechanics

This section introduces the field equations and corresponding state variables of the coupled boundary value problem of cardiac electromechanics.

2.1. Geometric mappings and the field variables

A *body B* is a three-dimensional manifold consisting of material points $\mathcal{P} \in B$. The motion of the body is defined by a one-parameter function of time via bijective mappings

$$\boldsymbol{\chi}(\mathcal{P},t) = \begin{cases} B & \rightarrow \quad \mathcal{B}(\mathcal{P},t) \in \mathbb{R}^3 \times \mathbb{R}_+, \\ \mathcal{P} & \mapsto \quad \mathbf{x} = \boldsymbol{\chi}_t(\mathcal{P}) = \boldsymbol{\chi}(\mathcal{P},t). \end{cases} \tag{1}$$

The point $\mathbf{x} = \boldsymbol{\chi}(\mathcal{P},t)$ denotes the configuration of the particle $\mathcal{P}$ at time $t \in \mathbb{R}_+$. Let the configuration of the material points at a reference time t_0 be denoted by $\mathbf{X} = \boldsymbol{\chi}(\mathcal{P},t_0) \in \mathbb{R}^3$ and $\boldsymbol{\chi}_t(\mathcal{P}) = \boldsymbol{\chi}(\mathcal{P},t)$ denote the placement map for a frozen time frame t. Then, the deformation map $\boldsymbol{\varphi}_t = \boldsymbol{\chi}_t \circ \boldsymbol{\chi}_0^{-1}(\mathbf{X})$ with

$$\boldsymbol{\varphi}_t(\mathbf{X}) = \begin{cases} \mathcal{B}_0 & \rightarrow \quad \mathcal{B} \in \mathbb{R}^3, \\ \mathbf{X} & \mapsto \quad \mathbf{x} = \boldsymbol{\varphi}(\mathbf{X},t), \end{cases} \tag{2}$$

maps the reference configuration $\mathbf{X} \in \mathcal{B}_0$ of a material point onto the spatial counterpart $\mathbf{x} \in \mathcal{B}$. The *deformation gradient*

$$\mathbf{F} : \mathbf{T}_X\mathcal{B}_0 \rightarrow \mathbf{T}_x\mathcal{B}; \quad \mathbf{F} := \nabla_X \boldsymbol{\varphi}_t(\mathbf{X}) \tag{3}$$

maps the unit tangent of the reference or the *Lagrangean* configuration onto its counterpart in the current or the *Eulerian* configuration. The gradient operators $\nabla_X[\bullet]$ and $\nabla_x[\bullet]$ denote the spatial derivative with respect to the reference $\mathbf{X}$ and current $\mathbf{x}$ coordinates, respectively. Moreover, the Jacobian $J := \det \mathbf{F} > 0$ characterizes the volume map of infinitesimal reference volume elements onto the associated spatial volume elements. Furthermore, the reference $\mathcal{B}_0$ and the spatial $\mathcal{B}$ manifolds are locally furnished with the covariant reference $\mathbf{G}$ and current $\mathbf{g}$ metric tensors in the neighborhoods $\mathcal{N}_X$ of $\mathbf{X}$ and $\mathcal{N}_x$ of $\mathbf{x}$, respectively. These metric tensors are required for the mapping between the co- and contravariant objects in the Lagrangean and Eulerian manifolds [31]. In order to impose the quasi-incompressible nature of the biological tissues, the deformation gradient $\mathbf{F}$ is decomposed into volumetric $\mathbf{F}_{vol} := J^{1/3}$ and unimodular $\bar{\mathbf{F}} := J^{-1/3}\mathbf{F}$ parts

$$\mathbf{F} = \mathbf{F}_{vol}\bar{\mathbf{F}}. \tag{4}$$

The ventricular myocardium is represented as a continuum with a hierarchical architecture consisting of discrete interconnected